

201-14189



NATALIE_RUTHERFORD@fmc.com on 12/30/2002 11:24:10 AM

To: oppt.ncic@epamail.epa.gov, Rtk Chem/DC/USEPA/US@EPA
cc: Richard Hefter/DC/USEPA/US@EPA

Subject:

FMC Corporation actively supports the EPA HPV Challenge Program and is pleased to submit the cover letter, proposed test plans and robust summaries for the two chemicals sponsored for the year 2002:

- Methyl 3,3-dimethyl-4, pentenoate - - CAS No. 63721-05-1
 - Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate - - CAS No. 64667-33-0

Please contact me if you have comments or questions regarding this submission.

Natalie Rutherford
Global Regulatory Manager
FMC Corporation

215-299-6680  DVE Step I Summaries 12-30.doc  DVE Step I Test Plan 12-30.doc
 DVE Step II Test Plan 12-30.doc  DVE Step I & II Cover Letter.doc  DVE Step II Summaries 12-30.doc

2002 DEC 30 PM 2:43

201-14189

2002 DEC 30 PM 3: 53

December 30, 2002

Administrator
US Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116
Attention: Chemical Right-to-Know Program

Registration Number:

Dear Administrator Whitman:

FMC Corporation actively supports the EPA HPV Challenge Program, AR-201 and is pleased to submit the proposed test plans and robust summaries for the two chemicals sponsored for the year 2002:

- Methyl 3,3-dimethyl-4, pentenoate - - CAS No. 63721-05-1
- Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate - - CAS No. 64667-33-0

FMC proposes Closed System Intermediate Status for both chemicals and information supporting exemption claims for Reduced SIDS Testing has been included in the robust summaries.

FMC understands there will be a 120-day review period for the test plan and that all comments received by EPA will be forwarded to FMC for consideration. Please contact me if you have comments or questions regarding this submission.

Sincerely,

Natalie Rutherford
Global Regulatory Manager
FMC Corporation
Tel. 215.299.6680
Fax 215.299.6468

DV Ester Step II (methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate), FMC 30099
CAS No. 64667-33-0

Study	Information (Y/N)	EPA/OECD Guideline (Y/N)	GLP (Y/N)	Other Study (Y/N)	Estimation Method (Y/N)	Acceptable (Y/N)	SIDS Testing Required (Y/N)
Physical and Chemical Data							
Melting Point	No	No	No	No	No	No	Yes
Boiling Point	Yes	No	No	No	No	No	Yes
Vapor Pressure	Yes	No	No	No	No	No	Yes
Partition Coefficient	No	No	No	No	No	No	Yes
Water Solubility	No	No	No	No	No	No	Yes
Environmental Fate and Pathways							
Photodegradation	Yes	No	No	No	Yes	Yes	No
Stability in Water (Hydrolysis)	Yes	No	No	No	Yes	Yes	No
Transport/Distribution	Yes	No	No	No	Yes	Yes	No
Biodegradation	No	No	No	No	No	No	Yes
Ecotoxicity							
Acute/Prolonged Toxicity to Fish	Yes	Yes	No	No	No	Yes	No
Acute Toxicity to Aquatic Invertebrates (Daphnia)	No	No	No	No	No	No	Yes
Acute Toxicity to Aquatic Plants (Algae)	No	No	No	No	No	No	Yes
Toxicity							
Acute Oral	Yes	Yes	Yes	No	No	Yes	No
Acute Dermal	Yes	No	Yes	No	No	Yes	No
Acute Inhalation	Yes	No	Yes	No	No	Yes	No
Repeated Dose	No	No	No	No	No	No	No
Genetic - Gene Mutation	Yes	No	Yes	No	No	Yes	No
Genetic - Chromosomal Aberration	No	No	No	No	No	No	Yes
Reproduction/Developmental Screen (OECD 421) ¹	No	No	No	No	No	No	Yes
Reproduction	No	No	No	No	No	No	No
Developmental/Teratogenicity	No	No	No	No	No	No	No

¹ Acceptable for satisfying Developmental Toxicity requirement for closed-system intermediates.

1. GENERAL INFORMATION

1.1 NUMBER 64667-33-0

1.2 CHEMICAL NAME Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate

1.3 EXPOSURE (CLOSED SYSTEM)

1.3.1. PROCESS DESCRIPTION

DVEster Step II is produced at the B-34 facility in the FMC Baltimore Plant.

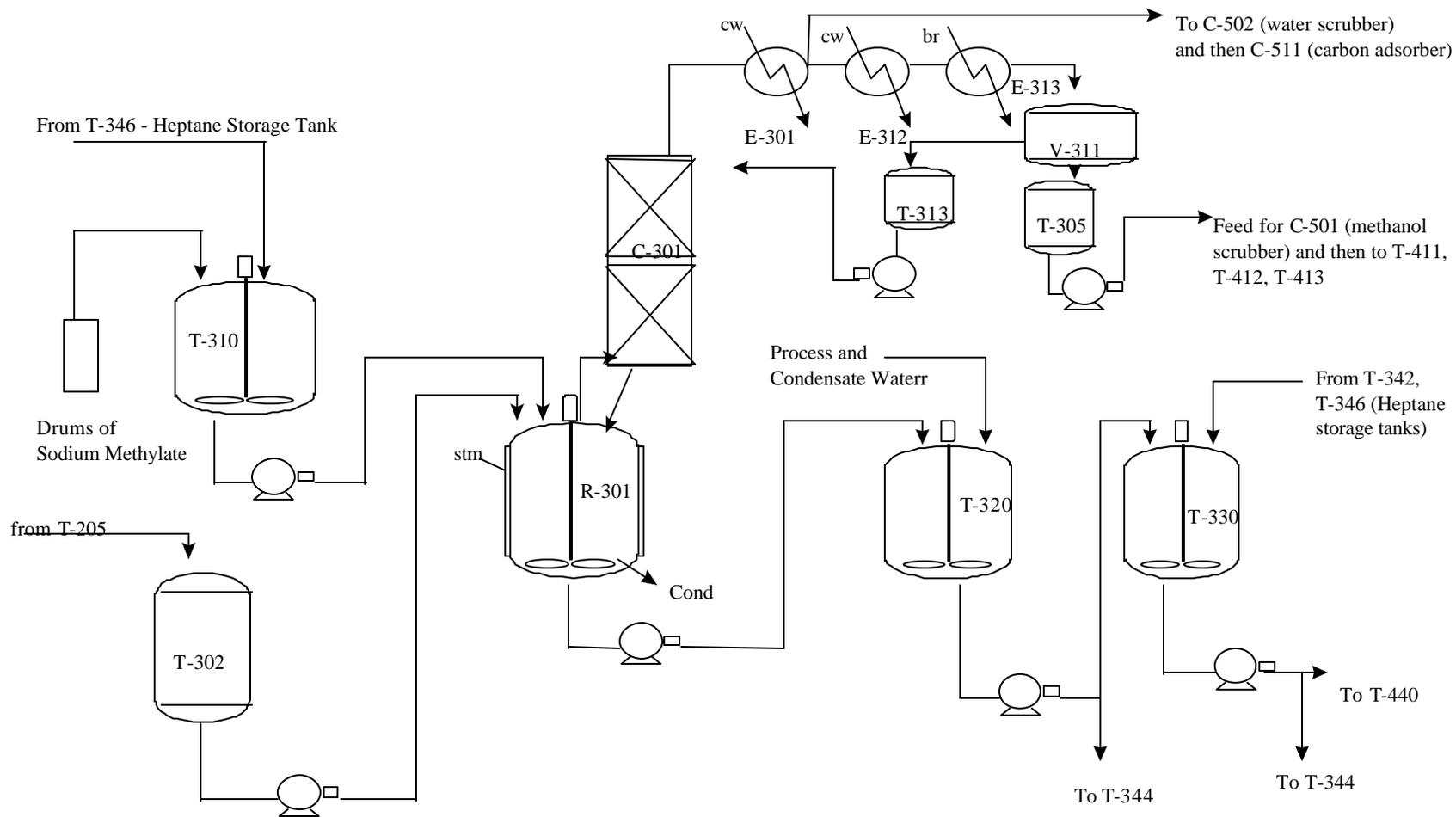
DVEster Step II product (FMC 30099) is produced by the reaction between Step I product (FMC 30098) and carbon tetrachloride (CCl₄) in the presence of a catalyst, benzoyl peroxide (BPO). See Figure 1 below.

Carbon tetrachloride is atmospherically stripped out of the reaction mass. Then a vacuum strip is performed to remove residual carbon tetrachloride and reaction by-products. The Step II product is then transferred to storage.

Step II product (FMC 30099) and sodium methylate are reacted to produce DVester (FMC 39338) in a batch reaction. Figure 2 shows the Step III reaction system. An excess sodium methylate/heptane slurry is mixed in T-310 and then fed to the reactor (R-301). After the slurry is heated, the reaction begins when Step II product is fed to the reactor.

The Step II product is converted to DVester through a series of irreversible dechlorination reactions. Two chlorines must be removed from the Step II before it becomes DVester. A total of 97-98% of the Step II is converted to DVester with the remaining percentage having only one chlorine removed (i.e, no longer existing as Step II material). The entire system is closed.

FIGURE 2
Step III Reaction and Wash System



T-205	T-310	T-301	E-301	E-313	V-311	T-320	T-330	T-440
Step II Product Storage Tank	Sodium Methylate Slurry Charge Tank	Step III Reactor Column	Step III Reactor Condenser	Step III Reactor After Condenser	Step III Reactor Decanter	Step III Wash Tank	Step III Extraction Tank	Waste Water Storage Tank
	T-302	R-301	E-312	T-313	T-305	T-344	T-411, 412, 413	
	Step III Product Feed Tank	Step III Reactor	Step III Chiller	Reflux Surge Tank	Waste Methanol Surge Tank	Heptane Stripper Feed Tank	Waste Methanol Storage Tanks	

1.3.2. MONITORING DATA

Wastewater monitoring - Wastewater samples are taken before every pump down to the south plant carbon beds. The limit for Step II in the water is 25 ppm. In 2001, our average concentration of Step II in this wastewater stream was 14.8 ppm.

IH Data – IH monitoring conducted in 1985 and 1988 indicated non detectable levels of Step II product in air. The limit of detection for the monitoring at that time was 0.1 mg.

1.3.3. PRESENCE IN DISTRIBUTED PRODUCT

No Dvester Step II is present in the Dvester Finished Goods products .

1.3.4 TRANSPORT DATA

Step II DVester is not transported.

1.3.5 PRESENCE IN END USE PRODUCTS

Confidential Statements of Formula - DVEster Step II is not included on any Confidential Statement of Formula for the technical materials produced in Baltimore using DVEster Step III Finished Goods as a raw material.

Literature Search - Results from a Chemical Abstracts On-line Database literature search indicate that DVEster Step II is not present in other end-products.

2. PHYSICAL AND CHEMICAL DATA

2.1 MELTING POINT

No data available.

2.2 BOILING POINT

2.2.1. SOURCE #1

Test Substance:

Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate

Method:

Unknown

GLP:

No

Year:

1978

Results:

110 - 114 ° C @ 93.3 Kpa (0.7 mm Hg)

Data Quality:

4e

References: "Permethrin Compendium", M. Fishman, November 17, 1980

2.2.2 SOURCE #2

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate

Method: Vacuum distillation

GLP: No

Year: 1999

Results: 101-103 ° C @ 0.1 mm Hg

Data Quality: 4e

References: Synthetic Communications 29(10), 1653-1659 (1999)

2.3 VAPOR PRESSURE

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, 100% pure

Method: Unknown

GLP: No

Year: Unknown

Results: 0.6 mm Hg @ 100°C

Data Quality: 4e

References: FMC MSDS

2.4 PARTITION COEFFICIENT

No data available.

2.5 WATER SOLUBILITY

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method: Unknown
GLP: No
Year: Unknown
Results: Insoluble
Data Quality: 4e
References: FMC MSDS

3 ENVIRONMENTAL FATE AND PATHWAY

3.1 PHOTODEGRADATION

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method: Estimated by the AOP program (v. 1.90) which estimates rate constants and half-lives of atmospheric reactions of organic compounds with hydroxyl radicals and ozone in the atmosphere.
GLP: No
Year: 2000
Results: For reaction with hydroxyl radicals, the predicted half-life is 5.2 days with a rate constant of 2.04×10^{-12} cm³/molecule-sec.
Remarks: The photodegradation calculation by an acceptable method is assigned a reliability code of 2f.
References: AOPWIN version 1.90, Syracuse Research Corporation, Syracuse, NY

3.2 STABILITY IN WATER (HYDROLYSIS)

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method: Estimated by HYDROWIN program (v. 1.67)
GLP: No
Year: 2000
Results: The predicted half-life is 5.4 years at pH 8 and 54 years at pH 7.
Remarks: The hydrolysis calculation by an acceptable method is assigned a reliability code of 2f.
References: HYDROWIN version 1.67, Syracuse Research Corporation, Syracuse, NY

3.3 TRANSPORT/DISTRIBUTION (FUGACITY MODEL)

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method: Estimated by EPI Suite program (v. 3.05)
GLP: No
Year: 002
Results: Distribution using Level III Fugacity model

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.67	125	1000
Water	9.71	3.6e+003	1000
Soil	72	3.6e+003	1000
Sediment	17.6	1.44e+003	0

Remarks: The fugacity calculation by an acceptable method is assigned a reliability code of 2f.
References: EPI Suite version 3.05, Syracuse Research Corporation, Syracuse NY

3.4 BIODEGRADATION No data available.

4 ECOTOXICOLOGY

4.1 ACUTE TOXICITY TO FISH

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method:	EPA, 1975, Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. Ecological Research Series EPA-660/3-75-009. 61 p. Test was conducted under static condition in 19 L uncovered jars which contained 15 L of natural, filtered (5 micrometers) sea water. Salinity was 17 parts per thousand. Temperature was maintained at 20 °C +/- 1. Initial pH was 8 +/- 0.5 for all test concentrations and controls. The sheepshead minnows measured 7 – 12 mm in standard length. Mortality was <3% during a 7-day acclimation period. The fish appeared to be in excellent condition at initiation of the test. Each test jar contained 10 fish. There was no aeration. Based on preliminary tests, sheepshead minnows were exposed to five concentrations of the test material. Test material was dissolved in reagent grade acetone and pipetted into sea water in the appropriate test containers to obtain the desired concentrations. A vehicle control was run with a volume of acetone equal to that added to the highest test concentration.
Species:	Sheepshead minnow (<i>Cyprinodon variegates</i>)
Test Concentration (nominal):	Control (0), 1.8, 3.2, 5.6, 7.5 and 10 ppm
Exposure Period:	96 hours
Analytical Monitoring:	No
GLP:	No
Year:	1976
Results:	The estimated 96-hour LC50 for sheepshead minnows in static, unaerated sea water was greater than 3.2 ppm but less than 5.6 ppm. Dissolved oxygen remained >65% of saturation in all test concentrations and controls for the duration of the test. The final pH was 8 +/- 0.5 for all test concentrations and controls.
Conclusion:	The 96-hour LC ₅₀ was between 3.2 and 5.6 ppm.

Data Quality: 2d

References: Acute Toxicity of four compounds to Sheepshead Minnows (*Cyprinodon variegates*), EG&G, Bionomics, FMC Study Number ACT 015.11-03, April 1976.

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES No data available.

4.3 TOXICITY TO AQUATIC PLANTS No data available.

5 TOXICITY

5.1 ACUTE TOXICITY

5.1.1 ORAL

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, purity > 97%

Method: US EPA Pesticide Assessment Guidelines; Subdivision F, Hazard Evaluation: Human and Domestic Animals, November, 1982; 81-2 Acute Oral Toxicity Study.

Ten rats (5 male and 5 female) were orally dosed with undiluted test material at a dosage of 5000 mg/kg. Observations for toxicity were conducted at 0.5, 1, 2, 3, 4 and 6 hours post-dosing and twice daily thereafter for thirteen days. On day 14, observations were only performed once. Body weights were recorded on days 0, 7 and 14 of the study. Gross necropsy was performed on all animals.

Species/strain: Sprague-Dawley

Sex: Male and Female

No. Animals/Group: 5/sex/group

Dose: 5000 mg/kg

Post-dosing observation period: 14 days

GLP: Yes

Year: 1984

Results: There were no deaths. Predominant clinical signs included abdominogenital staining, diarrhea, exophthalmos, lacrimation, decreased locomotion, nasal discharge and oral discharge. All signs subsided by day eight of the study. All surviving animals gained weight by day 14 of the study. There were no gross lesions in any animal at gross necropsy.

Conclusion: The test material is classified as practically non-toxic with a LD50 greater than 5000 mg/kg for both male and female rats.

Data Quality: 1

References: Acute Oral Toxicity of FMC 30099 Technical in Rats, FMC Study Number A1984-1459, July 29, 1985.

5.1.2 DERMAL

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, purity >97%

Method: The test substance was applied topically to the backs of 10 rabbits, 5 rabbits per dosage, under occluded conditions for 24 hours. Observations for toxicity were conducted daily, irritation was evaluated after 1, 2, 3, 4, 7 and 14 days.

Species/strain: New Zealand White Rabbits

No. Animals: 5 animals/group

Dose: 423 mg/kg and 28.2 mg/kg

Vehicle: None

Exposure Period: 24 hours

Post-exposure observations: Observations for toxicity: daily
Observations for irritation: 1, 2, 3, 4 and 7 days

GLP: Yes

Year: 1985

Results: There were no deaths. All rabbits remained healthy throughout the study. No treatment-related weight change was observed. Slight erythema and desquamation were noted sporadically. No gross lesions were observed at necropsy.

Conclusion: The test substance was practically non-toxic and minimally irritating.

Data Quality: 2c

References: Preliminary Dermal Toxicity/Irritation of FMC 30098 Technical in Rabbits, FMC Toxicology Laboratory, FMC Study A84-1419, April 25, 1985.

5.1.3 INHALATION

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, purity > 97%

Method: Five male and five female rats were exposed to the vapor of the test material for six hours at a nominal concentration of 5.5 ppm in a dynamically-operated, whole-body inhalation exposure chamber. Observations for toxicity and mortality were performed frequently during the exposure, upon removal from the chamber, at one hour post-exposure, and daily thereafter for fourteen days. Individual body weights were recorded immediately prior to exposure (day 0) and on days 7 and 14. On day 14, all animals were sacrificed and complete gross necropsy examinations were performed.

Species/strain: Sprague-Dawley

No. Animals: 5/sex/group

Dose: 5.5 ppm

Vehicle: undiluted

Exposure Period: 6 hours

Post-exposure observation period: 14 days

GLP: Yes

Year: 1987

Results: There were no deaths during the study. Clinical signs noted among test rats during the first hour of exposure included irregular breathing patterns and one rat had red periocular fur around the left eye at

removal. One of the control rats had perinasal fur upon removal from the chamber. Body weight changes occurred in the usual manner. No internal gross lesions were noted in any animal at necropsy.

The airborne concentration which represented essentially saturated vapors of the test substance was low and produced only a transient toxic response, suggestive of irritation during expose.

Conclusion: The inhalation LC₅₀ was greater than 5.5 ppm.

Data Quality: 2c

References: FMC 39008 Technical, Acute Inhalation Toxicity Screen in Rats, FMC Toxicology Laboratory, FMC Study A85-1660, July 10, 1987.

5.2 REPEATED DOSE TOXICITY No data available.

5.3 GENETIC TOXICITY IN VITRO AND IN VIVO

5.3.1 GENE MUTATION

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, Purity > 97%

Method: *Salmonella typhimurium*/Mammalian Microsome Plate Incorporation Mutagenicity Assay (Ames Test). The test was conducted using *Salmonella typhimurium* tester strains TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation by rat liver microsomes, S9, using the standard protocol. Appropriate positive and negative controls were included in the assay.

The test article was solubilized in DMSO and serially diluted immediately before its use in the mutagenicity assay. Five doses of the test material were plated with all five tester strains with and without metabolic activation. All solvent controls and test article doses were plated in triplicate.

Type: In vitro mutagenicity in bacteria

System of Testing: *Salmonella typhimurium* TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation by Aroclor induced rat liver mic rosomes, S9.

Concentration: 10 to 10,000 ug/plate

Metabolic Activation: S9

GLP: Yes

Year: 1986

Results: The test material did not cause a positive response in any of the five tester strains with or without metabolic activation.

Data Quality: 1a

References: Salmonella/Mammalian-Microsome Plate Incorporation Mutagenicity Assay (Ames Test), FMC Genetic Toxicology Laboratory, FMC Study Number A84-1449, April 6, 1986.

**5.3.2 CHROMOSOMAL
ABERRATION**

No data available.

5.4 REPRODUCTIVE TOXICITY

No data available.

**5.5 DEVELOPMENTAL
TOXICITY/TERATOGENICITY**

No data available.

CRITERIA FOR RELIABILITY CODES

(Adapted from Klimisch et al 1997)

<u>Code of Reliability</u>	<u>Category or reliability</u>
1	Reliable without restriction
1a	GLP guideline study (OECD, EC, EPA, FDA, etc.)
1b	Comparable to guideline study
1c	Test procedure in accordance with generally accepted scientific standards and described in sufficient detail
2	Reliable with restrictions
2a	Guideline study without detailed documentation
2b	Guideline study with acceptable restrictions
2c	Comparable to guideline study with acceptable restrictions
2d	Test procedure in accordance with national standard methods with acceptable restrictions
2e	Study well documented, meets generally accepted scientific principles, acceptable for assessment
2f	Accepted calculation method
2g	Data from handbook or collection of data
3	Not reliable
3a	Documentation insufficient for assessment
3b	Significant methodological deficiencies
3c	Unsuitable test system
4	Not assignable
4a	Abstract
4b	Secondary literature
4c	Original reference not yet available
4d	Original reference not yet translated
4e	Documentation insufficient for assessment